

propyl-cannabinolic acid, methyl-boronate

Inchi: InChI=1S/C21H23BO4/c1-6-7-13-11-16-18(19-17(13)20(23)26-22(5)25-19)14-10-12(2)8-
InchiKey: QDUIEGDZAYBNKR-UHFFFAOYSA-N
Formula: C21H23BO4
SMILES: CCCc1cc2c(c3c1C(=O)OB(C)O3)-c1cc(C)ccc1C(C)(C)O2
Mol. weight [g/mol]: 350.22

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|------|----------------|
| log10ws | -5.26 | | Crippen Method |
| logp | 4.909 | | Crippen Method |
| rinpol | 2573.00 | | NIST Webbook |

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R487626&Units=SI>

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
rinpol: Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/33-126-5/propyl-cannabinolic-acid-methyl-boronate.pdf>

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